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13. ABSTRACT *(Maximum 200 words)*

Droplet collision was simulated using two computational approaches, namely front tracking and molecular dynamics. By using the front tracking technique, the collision sequence in different collision regimes was simulated, the history of pressure and viscous dissipation within the droplet was spatially resolved, and the energy partition among the various modes was identified. By using the molecular dynamics method, bouncing and coalescence were successfully simulated for the first time without the artificial manipulation of the inter-droplet gaseous film. Several flame dynamics problems were also simulated, including flame-vortex interaction and flamefront instability in large-scale flows. In particular, it was found that wrinkling of a flame surface in the presence of a vortex is very much influenced by the Landau-Darrieus instability instead of the motion of the vortex itself, and that the wrinkling due to large-scale flows can suppress the formation of small-scale instabilities.

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COMPUTATIONAL SIMULATION OF DROPLET COLLISION DYNAMICS

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Narrative

For the subject grant, computational research was conducted on the dynamics of droplet collision and flamefront motion. Accomplishments of these two projects are separately discussed in the following.

Droplet Collision Dynamics

Droplet collision was simulated using two computational approaches, namely front tracking and molecular dynamics. By using the front tracking technique, the collision sequence in different collision regimes was simulated, the history of pressure and viscous dissipation within the droplet was spatially resolved, and the energy partition among the various modes was identified. The difficulty with the front tracking approach is its failure to simulate the state at which the surfaces of the two impinging droplets break such that merging can be effected. Simulation for this state would require the grid resolution down to the atomic scale, together with the inclusion of atomic forces in the simulation.

In response to such an intrinsic difficulty with simulation based on continuum mechanics, simulation based on molecular dynamics was conducted. Consequently bouncing and coalescence were successfully simulated for the first time without the artificial manipulation of the inter-droplet gaseous film. Furthermore, splashing collision was also observed.

Flame Dynamics

Considerable efforts were expanded in the development of computational algorithms for the simulation of flame surfaces. The specific emphasis here is the recognition that much of previous efforts in flame simulation did not account for thermal expansion in crossing the flame front. Since heat release across the flame is significant, leading to substantial disparities in the gas density, assumptions of constant density flames are quantitatively inadequate in describing flame dynamics.

Furthermore, since density jump across and interface also induces the Landau-Darrieus instability, neglecting thermal expansion also physically falsifies the phenomena of interest.

Two front-tracking algorithms were developed. The first adopts the multi-fluid approach used for the droplet collision simulation. Specifically, in droplet collision there is a great density disparity between the gas and the liquid, which are separated by a sharp deformable interface. This is similar to the situation of a wrinkled flame sheet separating the high-density unburnt gas from the low-density burnt gas. The second algorithm emphasizes the need for a sharp interface, recognizing that the interfaces in existing algorithms actually consist of several numerical grids and hence are not true discontinuities. The algorithm developed is believed to be the most accurate in the simulation of sharp interfaces.

By using these two algorithms, several flame dynamics problems were simulated, including flame-vortex interaction and flamefront instability in large-scale flows. In particular, it was found that wrinkling of a flame surface in the presence of a vortex is very much influenced by the Landau-Darrieus instability instead of the motion of the vortex itself, and that the wrinkling due to large-scale flows can suppress the formation of small-scale instabilities.

Publications

1. "A Front Tracking Method for the Motion of Premixed Flames," by J. Qian, G. Tryggvason, and C. K. Law, *Journal of Computational Physics*, Vol. 144, pp. 52-69 (1998).

2. "A Numerical Method for Solving Incompressible Flow Problems with a Surface of Discontinuity," by B.T. Helenbrook, L. Martinelli, and C.K. Law, *Journal of Computational Physics,* Vol. 148, pp. 366-396 (1999).

3. "The Role of Landau-Darrieus Instability in Large Scale Flows," by B.T. Helenbrook and C.K. Law, *Combustion and Flame,* Vol. 117, pp. 155-169 (1999).

4. "Molecular Simulation of Droplet Collision in the Presence of Ambient Gas," by S. Murad and C. K. Law, *Molecular Physics,* Vol. 96, pp. 81-85 (1999).